Metamagnetism in one dimensional systems with edge sharing CuO polihedra

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We study a Heisenberg chain with nearest-neighbor (NN) J_1 and next-NN J_2 exchange interactions with anisotropies Δ_1 and Δ_2 respectively. We investigate by analytical and numerical methods the region of parameters for which there is a jump in the magnetization M as a function of magnetic field B. Some materials with edge sharing CuO polihedra are candidates to show an abrupt change in $M(B)$.

The magnetization as a function of applied magnetic field in several materials [1–3] shows a discontinuity or very rapid increase at a certain field B_c. Gerhardt *et al.* have shown that for certain parameters, a magnetization jump is also present in the spin-1/2 XXZ chain with NN and next-NN exchange coupling (keeping $\Delta_1 = \Delta_2 = \Delta$) [4]:

$$H = \sum_i [J_1(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta_1 S_i^z S_{i+1}^z) + \sum_i J_2(S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta_2 S_i^z S_{i+2}^z)] - B\sum_i S_i^z, \tag{1}$$

For a metamagnetic transition to occur at very low temperatures, the zero-field ground-state energy per site E as a function of the magnetization $M = \sum_i S_i^z/L$ (L is the number of sites), should satisfy two conditions: I) $\partial^2 E/\partial M^2 < 0$ in a finite interval of values of M. Then one can draw a straight line $E'(M)$ which is tangent to $E(M)$ in at least two points (the Maxwell construction, see Fig. 1 (a)) in such a way that $E(M) \geq E'(M)$ for $M_1 \leq M \leq M_2$. II) $E(M_2) > E(M_1)$. If these two conditions are satisfied, M jumps from M_1 to M_2 at the critical field $B_c = [E(M_2) - E(M_1)]/(M_2 - M_1)$.

From the general behavior of $E(M)$, Gerhardt *et al.* have found that when metamagnetism exists, $M_2 = 1/2$ and the condition II ceases to be satisfied when $M_1 = 0$. More precisely, from their finite-size results for $E(M, \alpha, \Delta)$, with $\alpha = J_2/J_1$, they obtained a critical value of Δ ($\Delta_f(\alpha)$) from the equation $E(0, \alpha, \Delta_f) = E(1/2, \alpha, \Delta_f)$. For $\Delta < \Delta_f$ the system is ferromagnetic at $B = 0$. Another critical value $\Delta_a(\alpha)$ was obtained from the condition $\partial^2 E/\partial M^2|_{M=1/2} = 0$. For $\Delta > \Delta_a$ the curvature $\partial^2 E/\partial M^2$ is positive for all M. The discretized $\partial^2 E/\partial M^2|_{M=1/2} = 0$ has some finite-size effects [4]. From the numerical solution of the problem of two spin excitations on the ferromagnetic state for $L \to \infty$, more accurate values of $\Delta_a(\alpha)$ were obtained recently for $\alpha \leq 1/2$ [5]. In the region of the (α, Δ) plane where $\Delta_f(\alpha) < \Delta < \Delta_a(\alpha)$ a metamagnetic transition occurs in the model [4,5].

We have studied the two-magnon problem for generic values of Δ_1 and Δ_2, and found analytical results for the condition $\partial^2 E/\partial M^2|_{M=1/2} = 0$ if $\alpha \leq 0.75$. When $\Delta_1 = \Delta_2 = \Delta$, in the region $\alpha \leq 1/4$, the function $\Delta_f(\alpha)$ can be accurately approximated by:

$$\Delta_f = -1 + 2\sum_{i=1}^{4} \alpha^i + 6\alpha^5 + O(\alpha^6), \text{ if } \alpha \leq 0.2$$

$$\Delta_f = \frac{1}{4}(-5 + \sqrt{17}) - 0.462\sqrt{1 - 4\alpha}, \; 0.2 \leq \alpha \leq \frac{1}{4}.$$

For $1/4 \leq \alpha \leq 1/2$, although the algebra is more involved, the exact result is simpler:

$$\Delta_f = -b + \sqrt{b^2 - 2\alpha}, \text{ with } b = \alpha + \frac{1}{2} + \frac{1}{8\alpha}.$$

Finally in the region $1/2 \leq \alpha \leq 0.75$, $\Delta_f(\alpha)$ is very flat. Near $\alpha = 1/2$ it can be approximated as $\Delta_f = -\frac{1}{2} + 0.309(x - \frac{1}{2})^2$. These results show that metamagnetism is not possible if $\Delta > (-5 + \sqrt{17})/4 = -0.219$. Unfortunately, such a large anisotropy of J_2 seems unrealistic. Instead, $\Delta_1 = -1$ corresponds to isotropic ferromagnetic J_1, since a rotation of every second spin in π around the z axis changes the sign of the x and y components of J_1.

The main purpose of this work is to extend the previous results to negative Δ_1 and positive Δ_2. Since it is expected that the parameters for several copper oxides containing edge sharing Cu-O chains lie near the isotropic limit $\Delta_1 = -1$, $\Delta_2 = 1$, [6] we consider this limit in what follows. From numerical diagonalization of 20 sites, we obtain that spontaneous ferromagnetism does not take place for $\alpha > 1/4$. If in addition $\alpha \leq 0.7$, there is a bound state in the two-magnon problem at wave vector $q_2 = 2q_1$, where $q_1 = \pm \arccos[-1/(4\alpha)]$ are the wave vectors of the one-magnon states of lowest energy. For $\alpha > 0.7$, there might be a two-magnon bound state with $q_2 \neq 2q_1$, but we have not studied this alternative because it seems not possible to solve the problem analytically for large α. Thus, we expect a jump in $M(B)$ for $1/4 < \alpha \leq \alpha_c$ with $\alpha_c \geq 0.7$.

In Fig. 1(a) we show $E(M)$ for a chain of $L = 20$ sites with periodic boundary conditions for $\alpha = 0.425$, chosen in such a way that $q_1 = \pm 7\pi/10$ are allowed wave vectors of the finite chain. For other values of α, one

might obtain a numerical negative $\partial^2 E/\partial M^2|_{M=1/2}$ because of frustration effects which increase $E(M-1/L)$. In spite of this precaution, the results show a significant even-odd effect: the energies for odd (even) total spin $S=|M|L$ seem to be shifted to higher (lower) energies. If this effect persists in the thermodynamic limit (keeping L even) states with odd S become irrelevant (because they do not minimize $E-MB$ for any B) and a bound state in the two-magnon problem does not necessarily imply $\partial^2 E/\partial M^2|_{M=1/2}<0$. From $E(S/L)$ for the three highest even S with $L=28$, minimized with respect to the optimum twisted boundary conditions to allow for incommensurate wave vectors [7], we obtain a very small curvature which is negative for $\alpha<\alpha_c=0.359$ but positive for $\alpha>\alpha_c$. If α_c remains finite in the thermodynamic limit, $M(B)$ would increase abruptly for $\alpha>\alpha_c$, but without showing a true jump. While this difference is hard to distinguish experimentally, it would be of interest to calculate $\partial^2 E/\partial M^2|_{M=1/2}$ using larger clusters.

To obtain a continuous curve $E(M)$ from which $M(B)$ can be derived, we have fitted the eleven numerical values represented in Fig. 1(a) by a polynomial of even powers of M up to M^{10}. This function satisfies the physical condition $E(M)=E(-M)$ and has six fitting parameters (nearly half of the number of points to be fitted, to average the even-odd effect). The resulting $B=\partial E/\partial M$ is represented in Fig. 1(b). At a critical field $B_c=0.192J_1$, the magnetization jumps from $M_1=0.347$ to $M_2=1/2$. While the numerical values of B_c and particularly M_1 depend on the particular fitting procedure used and the size of the system, the general shape of $M(B)$ is robust: around $B/J_1=0.19\pm 0.01$ there is a sudden increase of M from ~ 0.25 to $1/2$. While the shape of $M(B)$ does not depend very much on $\alpha>1/2$, B_c increases strongly with α.

To conclude, while the existence of a real jump in $M(B)$ requires a study of larger clusters, we have shown that the magnetization of the model for parameters appropriate to edge-sharing Cu-O chains has a sudden increase at a magnetic field B_c. Using parameters calculated for $La_6Ca_8Cu_{24}O_{41}$, [6] and assuming a gyromagnetic factor $g=2$ we obtain $B_c\simeq 14$ Tesla.

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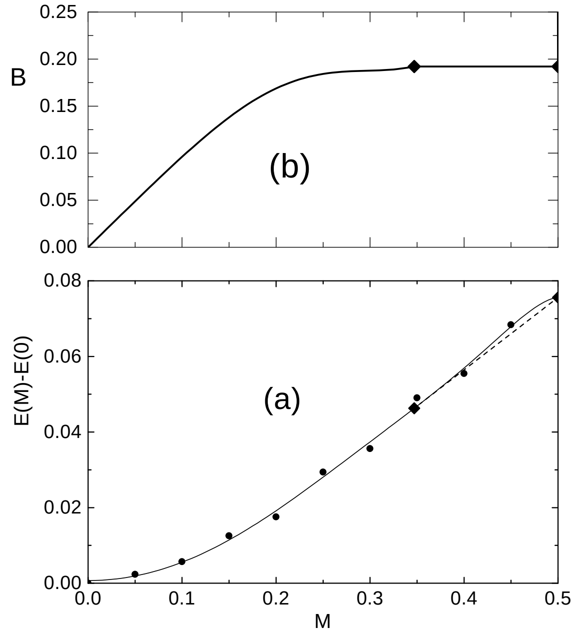

Fig. 1

FIG. 1. Energy per site as a function of total spin per site for a chain of 20 sites (solid circles). The full line is a fit (see text). Dashed line and diamonds correspond to the Maxwell construction. (b) Magnetic field as a function of the magnetization. Parameters are $J_1=1$, $J_2=0.425$, $\Delta_1=-1$ and $\Delta_2=1$.

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